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14. ABSTRACT

The purpose of this project has been to develop continuum phase-field models in concert with numerical methods for their solution to study dynamic brittle fracture. In contrast to discrete descriptions of fracture, phase-field descriptions do not require numerical tracking of discontinuities in the displacement field. This greatly reduces implementation complexity. During this project we have studied the basic formulations of the phase-field fracture theory, leading to second order partial differential equations (PDEs), along with the effect of adding higher-order

15. SUBJECT TERMS

brittle fracture, dynamic fracture, phase-field modeling, finite element modeling

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Chad Landis
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Report Title

Phase-field Modeling and Computation of Crack Propagation and Fracture

ABSTRACT

The purpose of this project has been to develop continuum phase-field models in concert with numerical methods for their solution to study dynamic brittle fracture. In contrast to discrete descriptions of fracture, phase-field descriptions do not require numerical tracking of discontinuities in the displacement field. This greatly reduces implementation complexity. During this project we have studied the basic formulations of the phase-field fracture theory, leading to second order partial differential equations (PDEs), along with the effect of adding higher-order gradients to the standard phase-field theory, leading to fourth and higher order PDEs. We have derived the thermodynamically consistent governing equations for the phase-field models by way of both balance law approaches and variational principles based on energy balance assumptions. We have completed studies on the implementation of second and fourth order phase-field methods for fracture brittle elastic materials as well as for fracture in brittle piezoelectric materials. We found that the fourth order phase-field model leads to higher regularity in the exact phase-field solution, which is exploited by the smooth function spaces utilized in isogeometric analysis. This increased regularity improves the convergence rate of the numerical solution and opens the door to higher-order convergence rates for fracture problems.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
04/07/2014	6.00	Michael J. Borden, Thomas J.R. Hughes, Chad M. Landis, Clemens V. Verhoosel. A higher-order phase-field model for brittle fracture: Formulation and analysis within the isogeometric analysis framework, Computer Methods in Applied Mechanics and Engineering, (05 2014): 100. doi: 10.1016/j.cma. 2014.01.016
04/07/2014	5.00	Zachary A. Wilson, Michael J. Borden, Chad M. Landis. A phase-field model for fracture in piezoelectric ceramics, International Journal of Fracture, (10 2013): 0. doi: 10.1007/s10704-013-9881-9
04/11/2012	2.00	Clemens V. Verhoosel, Michael A. Scott, Thomas J.R. Hughes, Chad M. Landis, Michael J. Borden. A phase-field description of dynamic brittle fracture, Computer Methods in Applied Mechanics and Engineering, (04 2012): 0. doi: 10.1016/j.cma.2012.01.008

TOTAL: 3

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

M.J. Borden, T.J.R. Hughes, C.M. Landis, M.A. Scott, C.V. Verhoosel, “Isogeometric analysis and phase-field modeling of dynamic linear elastic fracture mechanics.” Isogeometric Analysis 2011: Integrating Design and Analysis, Austin, Texas, January 2011.

M.J. Borden, T.J.R. Hughes, C.M. Landis, M.A. Scott and C.V. Verhoosel, “Phase-Field Modeling of Fracture”, McMat 2011, Chicago, IL. May 31, 2011.

M.J. Borden, T.J.R. Hughes, C.M. Landis, M.A. Scott, C.V. Verhoosel, “Isogeometric analysis and phase-field descriptions of crack propagation.” Computation Modeling of Fracture and Failure of Materials and Structures, Barcelona, Spain, June 2011.

M.J. Borden, T.J.R. Hughes, C.M. Landis, M.A. Scott, C.V. Verhoosel, “Isogeometric analysis of dynamic crack propagation using a phase-field model.” 11th US National Congress on Computational Mechanics, Minneapolis, Minnesota, July 2011.

M.J. Borden, T.J.R. Hughes, C.M. Landis, "Phase-field models for dynamic crack propagation in ductile material." Society of Engineering Science 49th Annual Technical Meeting, Atlanta, Georgia, October, 2012.

M.J. Borden, T.J.R. Hughes, C.M. Landis, "Phase-field models for dynamic brittle fracture." Society of Engineering Science 49th Annual Technical Meeting, Atlanta, Georgia, October, 2012.

Z.A. Wilson and C.M. Landis, “A phase-field approach to modeling crack propagation in piezoelectric ceramics.” ASME 2012 IMECE, Housotn, TX, November 2012.

C.M. Landis, M.J. Borden and T.J.R. Hughes, "Phase-field modeling of dynamic crack propagation." Workshop on the Design of Ceramic-Fiber Based Composites for Service Above 1400 Centigrade, Boulder, CO, June 2012.

M.J. Borden, T.J.R. Hughes, C.M. Landis, "Higher-order phase-field models for dynamic crack propagation." Advances in Computational Mechanics (ACM 2013), San Diego, California, February, 2013.

M.J. Borden, T.J.R. Hughes, C.M. Landis "Methods for improving convergence and accuracy of phase-field models for dynamic fracture in brittle and ductile materials." 12th US National Congress on Computational Mechanics, Raleigh, North Carolina, July, 2013.

M.J. Borden, T.J.R. Hughes, C.M. Landis, M.A. Scott, "Isogeometric analysis for higher-order damage and phase-field fracture models." Physics-Based Modeling in Design and Development for U.S. Defence Conference, Denver, Colorado, November, 2012.

Number of Presentations: 11.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
08/28/2013	3.00	Zachary A. Wilson, Michael J. Borden, Chad M. Landis. A Phase-Field Model for Fracture in Piezoelectric Ceramics, International Journal of Fracture (06 2013)
08/28/2013	4.00	Michael J. Borden, Thomas J.R. Hughes, Chad M. Landis, Clemens V. Verhoosel. A higher-order phase-field model for brittle fracture: Formulation and analysis within the isogeometric analysis framework, Computer Methods in Applied Mechanics and Engineering (07 2013)
08/29/2011	1.00	Michael J. Borden, Clemens V. Verhoosel, Michael A. Scott, Thomas J.R. Hughes, Chad M. Landis. A phase-field description of dynamic brittle fracture, Computer Methods in Applied Mechanics and Engineering (04 2011)

TOTAL: **3**

Number of Manuscripts:

Books

Received Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Honors for Thomas J.R. Hughes

World Class University Distinguished Invited Professor, School of Naval Architecture & Ocean Engineering, University of Ulsan, Ulsan, South Korea, September 25-October 23, 2010, March 4-20, May 11-20, August 8-26, 2011.

Elected a Foreign Member of the Royal Society, May 19, 2011. Inducted July 15, 2011.

ICES Grand Challenge Award, Institute for Computational Engineering and Sciences, University of Texas, Austin, Fall Semester, 2011.

Winston Chen Distinguished Lecture, Harvard School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts, October 19, 2011.

Fowler Distinguished Lecture, Department of Mechanical Engineering, Texas A&M University, College Station, Texas, November 16, 2011.

Joe J. King Professional Engineering Achievement Award, Cockrell School of Engineering, University of Texas, Austin, December 3, 2011.

John A. Blume Distinguished Lecture, Stanford University, Stanford, California, March 1, 2012.

Elsevier Distinguished Lecture in Mechanics, New Jersey Institute of Technology, Newark, New Jersey, April 11, 2012.

World Class University Distinguished Invited Professor, School of Naval Architecture & Ocean Engineering, University of Ulsan, Ulsan, South Korea, March 4-10, May 5-30, August 11-28, 2012.

In 2012 the Computational Fluid Mechanics Award of the United States Association of Computational Mechanics was renamed the
Thomas J.R. Hughes Medal.

"Isogeometric Analysis," Charlemagne Distinguished Lecture, Aachen Institute for Advanced Study in Computational Engineering
Science, (AICES), RWTH – Aachen University, Aachen, Germany, October 24, 2012.

ACM 2013, Advances in Computational Mechanics, A Conference Celebrating the 70th Birthday of Thomas J.R. Hughes, San Diego,
California, February 24-27, 2013.

World Class University Distinguished Invited Professor, School of Naval Architecture & Ocean Engineering, University of Ulsan, Ulsan,
South Korea, March 7-22, May 6-26, and August 9-26, 2013.

"Isogeometric Analysis," Raymond D. Mindlin Distinguished Lecture, Department of Civil Engineering and Engineering Mechanics, Davis
Auditorium, Shapiro Center, Columbia University, April 25, 2013.

"Isogeometric Methods: A Symposium Celebrating the 70th Birthday of Professor Thomas J.R. Hughes," USNCCM12, 12th U.S. National
Congress on Computational Mechanics, Raleigh, North Carolina, July 22-25, 2013.

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Zachary A. Wilson	0.50	
Michael J. Borden	0.50	
FTE Equivalent:	**1.00**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Michael J. Borden	0.50
FTE Equivalent:	**0.50**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Chad M. Landis	0.08	
Thomas J.R. Hughes	0.01	Yes
FTE Equivalent:	**0.09**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME	
Michael J. Borden	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attachment.

Technology Transfer

PHASE-FIELD MODELING AND COMPUTATION OF CRACK PROPAGATION AND FRACTURE

Scientific Progress and Accomplishments

PIs: Chad M. Landis and Thomas T.J.R. Hughes

Students: Michael J. Borden and Zachary A. Wilson

Aerospace Engineering and Engineering Mechanics
The University of Texas at Austin
210 East 24th Street, C0600
Austin, TX 78712-0235

I. Research Objectives

Over the past two decades research on the numerical simulation of fracture phenomena has progressed significantly and has had a tremendous impact on engineering practice and design. Important advances include the cohesive surface model, the virtual internal bond method, the extended finite element method, level set methods, and phase-field models for fracture. Of these approaches, the extended finite element and level set methods rely on established engineering fracture mechanics concepts, such as stress intensity factors or energy release rates, to determine when a crack will grow. Additional rules must then be implemented for the crack growth direction, e.g. maximum hoop stress or vanishing mode II stress intensity, and for crack nucleation. In contrast, the cohesive surface and virtual internal bond methods do not require any phenomenological rules for nucleation and growth. However, both of these methods suffer from numerical mesh-dependency. Depending on the method of implementation, cohesive surfaces can affect the overall elasticity of the structure and the crack path morphology. The phase-field approach appears to address both of these deficits, as it does not use any phenomenological rules for nucleation and growth and it contains a material length scale that mitigates any mesh-dependency. The arguable weakness of present phase-field approaches to fracture is the lack of a solid physical foundation for the damage parameter describing the degradation of the material. The research objectives of this project are to model fracture by integrating the strengths of the virtual internal bond and phase-field methodologies. Specifically, the phase-field fracture modeling approach will be implemented numerically to study a range of quasi-static and dynamic fracture problems. The physical veracity of the approach will be assessed through comparison with existing experimental benchmarks.

II. Approach

The novelty of the proposed approach includes the incorporation of physically based constitutive models into the phase-field fracture modeling framework and the implementation of the relatively new isogeometric numerical modeling and analysis technologies. The success of this program may enable entirely new solution procedures for important engineering problems that have heretofore proved intractable, such as, dynamic propagation of multiple cracks in three-dimensional bodies.

We have made significant progress on the following studies:

- Quasi-one-dimensional solutions where the model itself remains three-dimensional, but the solutions vary in only one direction. This study is important for describing the fundamental defect being modeled, the material surface, and for quantifying the surface energy within the model.

- Static simulations of initial crack propagation for a cracked body. These simulations are important to demonstrate that the theory agrees with classical Griffith theory, i.e. the crack should grow once the energy release rate reaches twice the surface energy.

- Dynamic crack growth studies have been performed to investigate crack tip speed, crack branching and crack interactions with free surfaces.

- Crack path selection during mixed mode loading and in isotropic materials.

- We have studied different approaches and phenomenology to generate fourth and higher order partial differential equations in the model, which are readily solved using isogeometric analysis technology. Preliminary investigations indicate that higher order theories may provide unforeseen benefits for the representations of crack surfaces.

III. Significance

In general, accurate models of crack nucleation, growth and interaction are critical for many Army applications. This is in fact the primary goal of the proposal, to develop a fundamental modeling approach for fracture. The methods developed provide a framework for multiple and in fact a very large number of cracks because crack formation is not tied to the geometry or topology of a numerical analysis mesh. Cracks may form anywhere spontaneously and their interaction is automatically accounted for. In this sense, the number of cracks is essentially unlimited, which may be thought of as a precursor to fragmentation. However, the problems of fragmentation and debris flow are clearly non-trivial. We envision that our modeling approach will serve as a prelude of the solution to those problems.

IV. Accomplishments in the current grant

The primary accomplishments during the present period of this grant are detailed in the three manuscripts listed in the Journal Articles section. We have extended a phase-field model for quasi-static brittle fracture to the dynamic case. We introduce a phase-field approximation to the Lagrangian for discrete fracture problems and derive the coupled system of equations that govern the motion of the body and evolution of the phase-field. We study the behavior of the model in one dimension and show how it influences material properties. For the temporal discretization of the equations of motion, we present both a monolithic and staggered time integration scheme. We study the behavior of the dynamic model by performing a number of two and three-dimensional numerical experiments. We also introduce a local adaptive refinement strategy and study its performance in the context of locally refined T-splines. We show that the combination of the phase-field model and local adaptive refinement provides an effective method for simulating fracture in three dimensions. The basics of the model are discussed very briefly here, and the reader is referred to the manuscripts for additional details.

Continuum Phase-Field Modeling Approach

The simplest phase-field model that can be used to model linear elastic fracture mechanics is presented. There are two approaches to the derivation of the governing partial differential equations for such models. One is a balance law approach where the constitutive behaviors of the specific material are separated from the fundamental balance laws (conservation of momenta, first and second laws of thermodynamics). A second approach is to construct a Lagrangian and then use the methods of Lagrangian mechanics. For either method the governing phase-field equations used to represent linear elastic fracture mechanics behaviors are as follows.

The Helmholtz free energy for the material is assumed to take the form,

$$\psi = \psi_{\varepsilon}^{-}(\varepsilon_{ij}) + c^2 \psi_{\varepsilon}^{+}(\varepsilon_{ij}) + G_c \left[\frac{(c-1)^2}{4l_0} + l_0 c_{,i} c_{,i} \right].$$

Here, the elastic part of the free energy has been decomposed into compressive, ψ_{ε}^{-}, and tensile, ψ_{ε}^{+}, parts. Notice that the "damage" parameter c only acts on the tensile part of the free energy. When $c \approx 1$ the material is intact and when $c \approx 0$ the material is failed. By only applying the phase-field parameter c to the tensile part of the elastic energy density, crack propagation under compression is prohibited. This model feature has been observed to be particularly important in dynamic simulations, as stress waves reflecting from boundaries can create physically unrealistic fracture patterns. The two new parameters introduced in the free energy are the fracture energy G_c, and the characteristic process zone length l_0. Homogeneous solutions of the theory can be obtained to yield the failure strength $\sigma_0 = \tfrac{9}{16}\sqrt{G_c E / 6l_0}$, where E is Young's modulus. To relate predictions of the phase-field theory to those from cohesive zone models, the characteristic critical opening displacement of the cohesive traction-separation law is $\delta_0 \propto G_c / \sigma_0 = \tfrac{16}{9}\sqrt{6 G_c l_0 / E}$.

Next, conservation of momentum (equilibrium for quasi-static simulations) in the volume and on surfaces leads to,

$$\left(\frac{\partial \psi}{\partial \varepsilon_{ij}} \right)_{,j} + b_i = \rho \ddot{u}_i \text{ in } V \text{ and } \frac{\partial \psi}{\partial \varepsilon_{ij}} n_j = t_i \text{ on } S.$$

As indicated above, the Helmholtz free energy of the material depends on the strain components, ε_{ij}, and the fracture order parameter, c. The body forces and surface tractions are b_i and t_i, and the mechanical displacement components are u_i. The components of the vector n_i are for the unit normal to the bounding surface S of the volume V. Linear kinematics is assumed such that, $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$. Next, the variational derivative of the Lagrangian, or equivalently a micro-force balance, provides the governing equation for the fracture order parameter as,

$$\left(\frac{\partial \psi}{\partial c_{,i}} \right)_{,i} - \frac{\partial \psi}{\partial c} = 0 \quad \rightarrow \quad 2 G_c l_0 c_{,ii} - 2\phi \psi_{\varepsilon}^{+} - \frac{G_c}{2l_0}(c-1) = 0.$$

Notice that the phase-field equation is second order in space and hence standard finite element approaches can be utilized for its solution. However, we are also studying higher order representations of the non-local term $G_c l_0 c_{,i} c_{,i}$ in the free energy which will require basis functions with higher than C0 continuity. Figure 1 below is an illustration of the types of results that are being obtained from the theory. This simulation is new and was not reported in the manuscript.

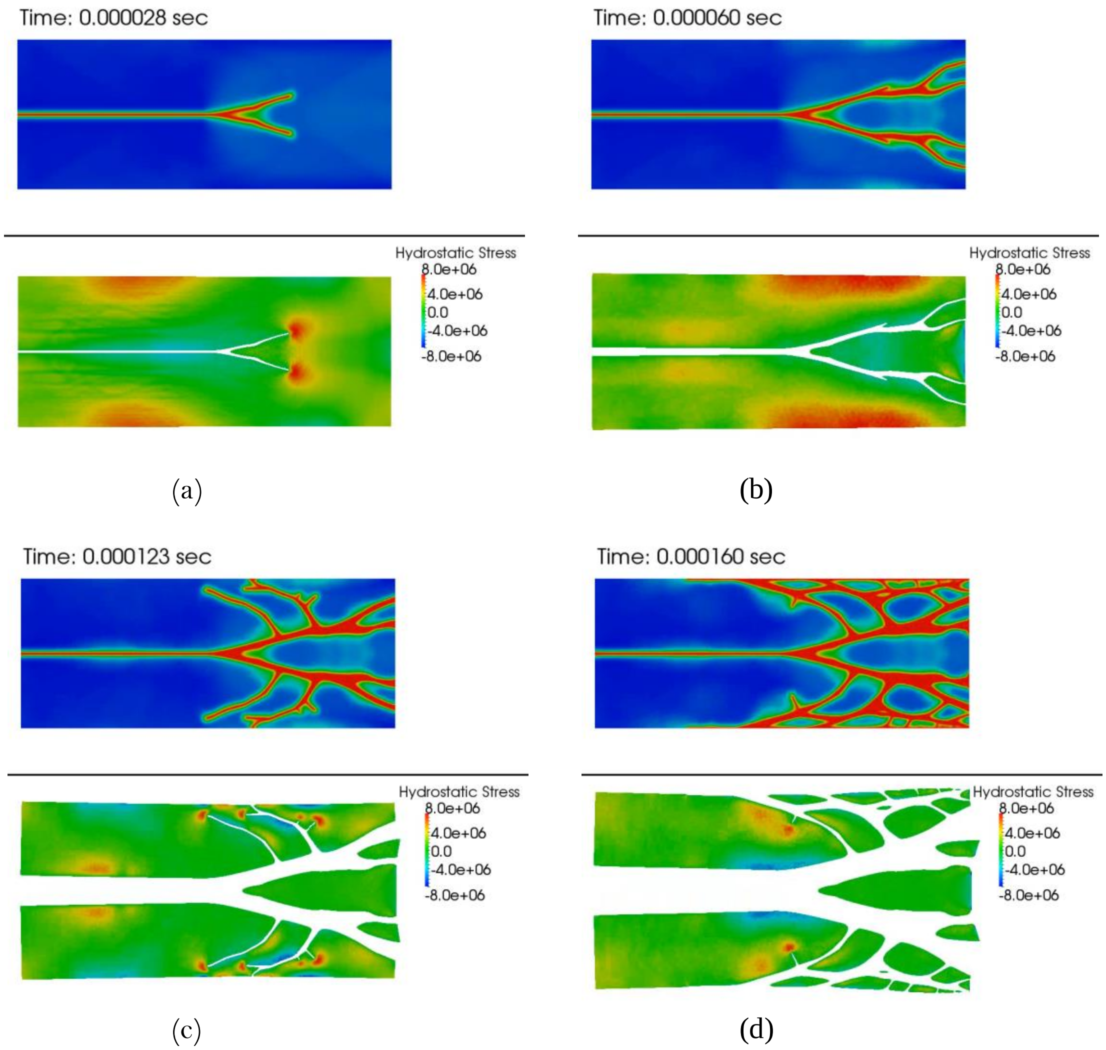
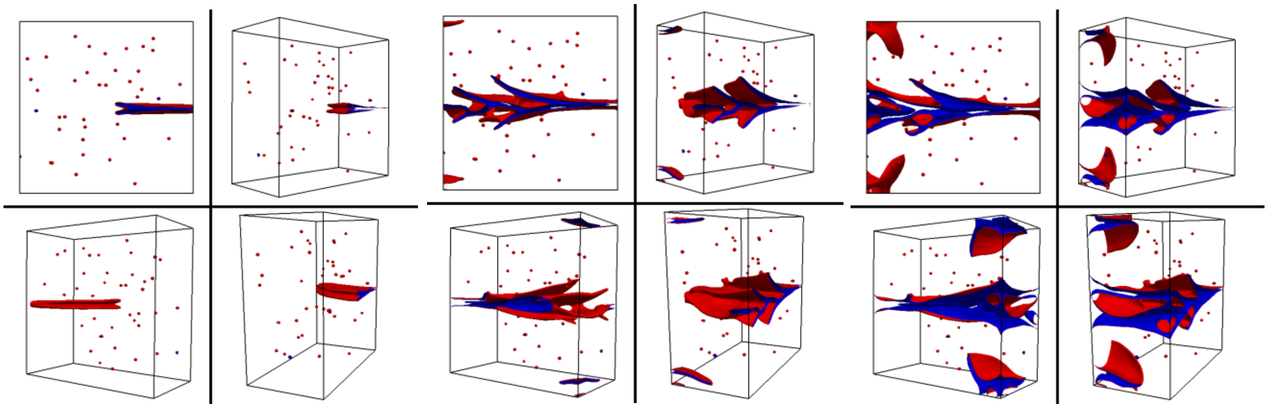


Figure 1. A two-dimensional example of the application of phase-field fracture modeling to dynamic, brittle fragmentation. The idealized model sample is a rectangular plate with an initial crack traversing through half of the centerline. Tensile tractions are applied on the top and bottom surfaces at time t=0 and held fixed through the duration of the simulation. Figures (a)-(d) illustrate snapshots at different times during the crack evolution process. The top contour plots show the phase-field variable with red indicating the location of the cracks and blue indicating intact material. The bottom contour plots show the distribution of hydrostatic stress superimposed on the deformed configuration of the sample. At the level of applied traction shown the crack undergoes (a) branching, (b) secondary branching, (c) initiation of multiple secondary cracks, and (d) the interaction of cracks and the creation of fragments.



(a) (b) (c)

Figure 2. A three-dimensional example of the application of phase-field fracture modeling to dynamic crack initiation and growth in a defected material (four viewpoints of the same box). Figures (a)-(c) illustrate (a) nucleation, growth and the onset of branching of an initial crack, (b) multiple branching of the initial crack and the nucleation of secondary cracks, and (c) evolution of the crack fronts and in particular the turning and twisting of 3D crack fronts. It is worth noting the very complex topology of the initial crack with one side of the crack being branched and the other side relatively smooth with a complex transition in the topology towards the middle.

In addition to these studies on brittle fracture in elastic materials we have also made progress on modeling fracture in piezoelectric materials, investigating the effects of a damage function that allows for nearly linear elastic behavior up to failure, and incorporating plasticity into the phase-field framework. Finally, we have also investigated a fourth-order model for the phase-field approximation of the variational formulation for brittle fracture. We derived the thermodynamically consistent governing equations for the fourth-order phase-field model by way of a variational principle based on energy balance assumptions. The resulting model leads to higher regularity in the exact phase-field solution, which can be exploited by the smooth spline function spaces utilized in isogeometric analysis. This increased regularity improves the convergence rate of the numerical solution and opens the door to higher-order convergence rates for fracture problems. We present an analysis of our proposed theory and numerical examples that support this claim. We also demonstrate the robustness of the model in capturing complex three-dimensional crack behavior.

V. Journal Articles

M.J. Borden, C.V. Verhoosel, M.A. Scott, T.J.R. Hughes and C.M. Landis, 2012, A Phase-field Description of Dynamic Brittle Fracture, *Computer Methods in Applied Mechanics and Engineering* **217-220** 77-95.

Z.A. Wilson, M.J. Borden, and C.M. Landis, 2013. "A Phase-field Model for Fracture in Piezoelectric Ceramics", *International Journal of Fracture* **183** 135-153.

M.J. Borden, T.J.R. Hughes, C.M. Landis, and C.V. Verhoosel, 2014. "A Higher-order Phase-Field Model for Brittle Fracture: Formulation and Analysis within the Isogeometric Analysis Framework", *Computer Methods in Applied Mechanics and Engineering* **273** 100-118.

VI. Graduate Students Involved Directly in ARO Project

Michael J. Borden (PhD earned 2012) and Zachary A. Wilson (currently enrolled)